Visualize the Difference

The Advanced Simulation and Computing (ASC) Program is a national program that enables the Department of Energy and National Nuclear Security Administration Stockpile Stewardship mission. ASC creates simulation tools to be used in concert with expert scientific judgment to certify that the stockpile is safe, reliable, and secure.

Cover:
Los Alamos RAGE simulation of a supersonic jet experiment on the OMEGA laser, designed to validate turbulent mix models.

As a program, ASC's main goal is to enable Stockpile Stewardship by:

- Improving the confidence in prediction through simulations
- Integrating the ASC Program with certification methodologies
- Developing the ability to quantify confidence bounds on the uncertainty of our results
- Increasing predictive capability through the development of more accurate physics and engineering models and tighter integration of simulation and experimental activities
- Providing the necessary computing capability to code users, in collaboration with industrial partners, academia, and government agencies

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For more information, visit http://www.sandia.gov/NNSA/ASC/

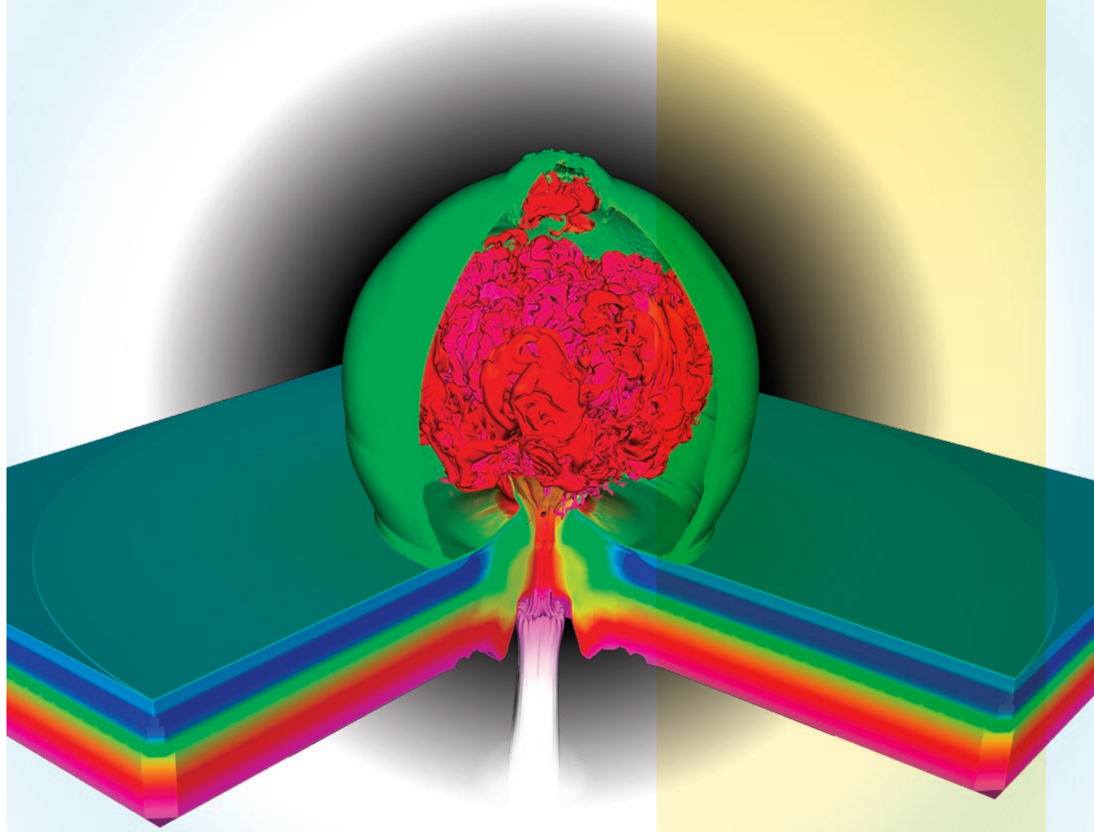
NNSA National Nuclear Security Administration

Lawrence Livermore National Laboratory

Los Alamos NATIONAL LABORATORY EST. 1943

Sandia National Laboratories

Advanced Simulation & Computing



Visualize the Difference

Predict, with confidence, the behavior of nuclear weapons through comprehensive, science-based simulations

ASC™

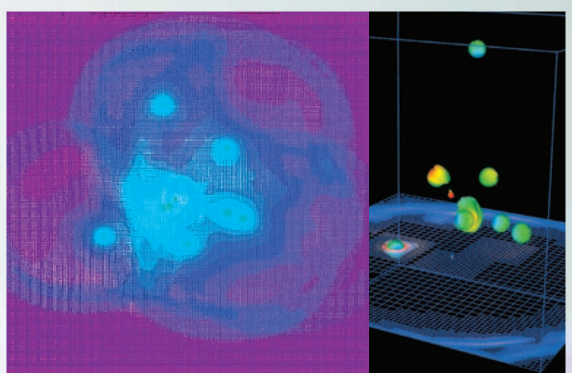
Platforms Tailored to Mission Goals

Capacity Computing

Capacity computing is accomplished through the use of smaller and less expensive high-performance systems to run parallel problems with more modest computational requirements.

Linux-based clusters are now being used for ASC capacity computing work at Lawrence Livermore, Los Alamos, and Sandia National Laboratories to provide cost-effective computational resources and a stable environment for weapons design and certification applications. The Linux-based clusters include systems such as Lightning at Los Alamos, Lilac and ALC at Livermore, and Thunderbird at Sandia. To keep costs low, ASC is leveraging commodity components, the Linux operating system, and a variety of open source software for tools, system monitoring and control, job scheduling, and file systems. The systems typically are used for problems that require hundreds of processors or a few thousand, not many thousands. Currently, ASC provides users across the program almost 200 teraOPS (two-hundred-trillion floating-point operations per second) of capacity computing power.

Lightning Linux cluster systems at Los Alamos National Laboratory, have 4,736 dual-processor AMD Opteron nodes with a Myrinet interconnect and a peak speed of 43 teraOPS. Lightning has 235 terabytes of temporary high-speed parallel storage and enjoys an award-winning architecture developed at Los Alamos (Science Appliance) and a software suite (Clustermatic) that can completely control a cluster.



Computational hydrodynamics, the application of supercomputing modeling to the behavior of liquids and gases in motion, applies to behavior in both terrestrial and cosmic settings and has been used to study many physical processes, including conduction, viscosity, shock waves, radiative transfer, and turbulence. Shown here is column density (the areal density along the line of sight) from a model of the central region of the galaxy. The round spots in the image are stars orbiting the central supermassive black hole. Shocks due to winds from these stars can be seen as bubbles expanding through the interstellar medium. The calculation used the ASC RAGE code developed by Los Alamos and SAIC and was run on FLASH, an ASC Linux cluster at Los Alamos.

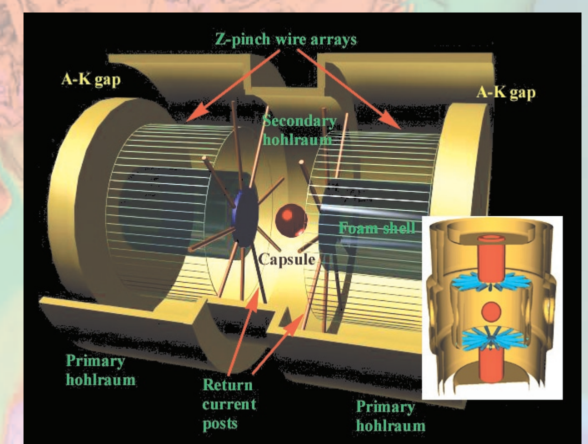
Capability Computing

Capability computing refers to the use of the most powerful supercomputers to solve the largest and most demanding problems with the intent to minimize time to solution. A capability computer is dedicated to running one problem, or at most a few problems, at a time.

The new capability computers ASC Purple at Lawrence Livermore and ASC Red Storm at Sandia will solve multiscale, multiphysics problems for the nation's Stockpile Stewardship Program—a program for maintaining the safety and reliability of the nation's nuclear weapons. The Stockpile Stewardship Program integrates the activities of the U.S. nuclear weapons complex, which includes the three defense laboratories as well as four production sites and the Nevada Test Site. As the nuclear weapons in the stockpile continue to age, laboratory scientists and engineers must ensure their performance and refurbish them as necessary without conducting nuclear tests.

The Red Storm supercomputer, at 40 teraOPS, represents a highly balanced and integrated capability machine well-suited to running a mix of weapons performance, stockpile science, and engineering applications.

Between its 94 teraOPS classified and its 6 teraOPS unclassified environment, ASC Purple will achieve the major milestone set in 1996 for a one-hundred-teraOPS-class computer dedicated to 3D capability computing.



Inertial Confinement Fusion (ICF) concepts for ignition, high yield, and fusion energy production are a focus of the Pulsed Power Sciences Center's Z experimental facility at Sandia. For example, the Double-Ended Hohlraum is an ICF concept with an inherently 3D cylindrical array of hundreds of discrete fine wires. When energized, the array implodes and generates a radiation source that absorbs and reflects off the walls to produce a "radiation bath," which in turn brings the target capsule to fusion conditions. ASC capability computers, running ASC codes like ALEGRA-HEDP, are required to simulate the 3D nature of the wire array and the radiation field. These simulations depend on a variety of complex material models for experimental and mission-critical materials. Predictive design and analysis simulation tools are essential to enable the productive use of this facility for experiments to meet the needs of ICF and the Science Campaigns.

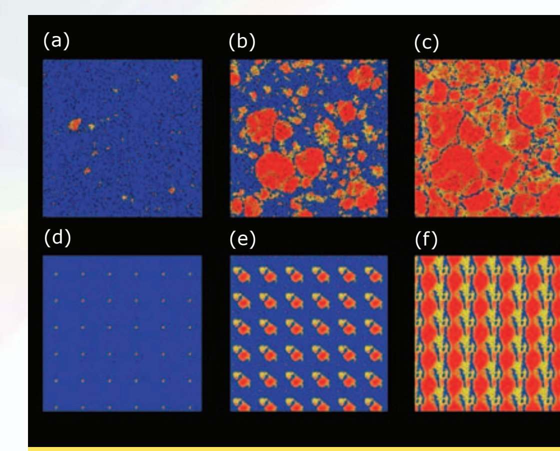
Advanced Systems

ASC invests research and development dollars in problem-optimized systems in response to programmatic needs. This includes cost-effective computers designed to achieve extreme speeds in addressing specific stockpile issues. Often, programmatic needs require the simultaneous development of enhanced performance codes that will run well on these new systems.

In late August, scientists at Lawrence Livermore and Los Alamos had an opportunity to run at full scale on BlueGene/L. Running on all 131,072 processors, the molecular dynamics code ddcMD achieved a world-record performance of 101.5 teraOPS sustained over seven hours. Along with ddcMD, the Qbox code from Livermore and the SPaSM code from Los Alamos achieved very high, sustained-rates computation. All three are finalists for the prestigious 2005 Gordon Bell Prizes for high-performance computing.

The ddcMD molecular dynamics code achieved its unprecedented performance while calculating the quench process in a molten actinide system. This was the largest simulation ever attempted using quantum-based MGPT interaction potentials and demonstrates that the BlueGene/L architecture can scale with real-world applications. Previous ddcMD calculations on BlueGene/L investigated solidification in tantalum, a transition metal. The simulations are significant because nucleation and growth of solids from a liquid are common phenomena that are well-studied but not very well understood. New insights into the solidification of metals are important to stockpile stewardship but can also yield benefit for a wide variety of industrial design and manufacturing applications.

BlueGene/L is an example of an ASC Advanced System. This machine is well-suited to run molecular dynamics applications at extreme speeds to address materials aging issues confronting the Stockpile Stewardship Program. BlueGene/L is also used to explore the potential of system-on-a-chip technologies to achieve extreme speed while minimizing floor space and electrical power consumption.



Snapshots from simulations of solidification in tantalum. The top sequence displays nucleation (a) and growth (b) occurring in a 16,372,000-atom simulation, resulting in a realistic distribution of grains and grain boundaries (c). The same process modeled using 64,000 atoms (d–f) produced the artificial final structure shown in (f).